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Modelling of a microelectromechanical thermoelectric cooler

F. Völklein [a,*], Gao Min [b], D.M. Rowe [b]

[a] University of Applied Sciences Wiesbaden, Germany
[b] School of Engineering, University of Wales Cardiff, Cardiff, UK

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Abstract

We represent the modelling of a thermoelectric cooler, which is designed by using micromachining and thin film technology. The cooler fabrication is compatible with standard semiconductor technology. Therefore, it can be integrated in microelectronic circuits. The most important parameters of the device like cooling power, maximum temperature difference and optimum current density are calculated. By using thermoelectric thin films with high efficiency and very thin SiC/Si_3N_4-membranes, a cooling power of a few milliWatts or maximum temperature difference of 30–50 K can be achieved.

Keywords: Thermoelectric microcooler; Modelling; Microelectromechanical system; Dew-point sensor

1. Introduction

Thermoelectric coolers (Peltier devices) are widely employed in microelectronics to stabilize the temperature of laser diodes, to cool infrared detectors and charge-coupled devices (CCD), and to reduce unwanted noise of integrated circuits.

A conventional thermoelectric cooler usually consists of a number of n- and p-type bulk semiconductor thermoelements connected electrically in series by metallizations and sandwiched between two electrically insulating but thermally conducting ceramic plates [1]. The dimensions of commercially available coolers varies from about $4 \times 4 \times 3$ to around $50 \times 50 \times 5$ mm^3. Although in principle, the dimensions can be reduced further, the preparation of conventional thermoelectric coolers is a bulk technology and is incompatible with microelectronics fabrication processes.

Thin film thermoelectric devices with very small dimensions have been fabricated using microelectronics technology as generators [2] and sensors for radiation [3,4], electrical AC and DC power [5–8], flow [9] and low vacuum [10,11]. However, to date, such thermoelectric devices have not been used successfully as thermoelectric coolers because the substrate is thick compared to the thin film thermoelements. Consequently, the cooling achieved by the device, when operated in the Peltier mode, is drastically reduced by the substrate's thermal bypass [12–14].

Recently, we have developed very thin SiC/Si_3N_4-membranes (200 nm thick) with compensated mechanical stress on bulk silicon wafers. These membranes are prepared by PECVD of the SiC/Si_3N_4 films and by micromechanical anisotropic etching of the silicon wafer from the backside. The small thermal bypass of these membranes facilitates the fabrication of a thin film thermoelectric cooler with sufficient cooling power and temperature difference. We report on the modelling of such microelectromechanical coolers.

2. Thermal model of the thermoelectric cooler

Fig. 1 shows the top view and cross-sectional view of the thermal model. The cooler consists of a number n of thermocouples connected in series (thermopile) and arranged with their cold junctions (temperature T_c) around the cooled area F, whereas their hot junctions are in good thermal contact with the heat sink. The thermopile and the cooled area are supported by a very thin membrane with

* Corresponding author. FHW Fachbereich Physikalische Tech., Am Bruckweg 26, 65428 Russelheim, Germany. Tel.: +49-46-6142-898-531; Fax: +49-46-6142-898-528

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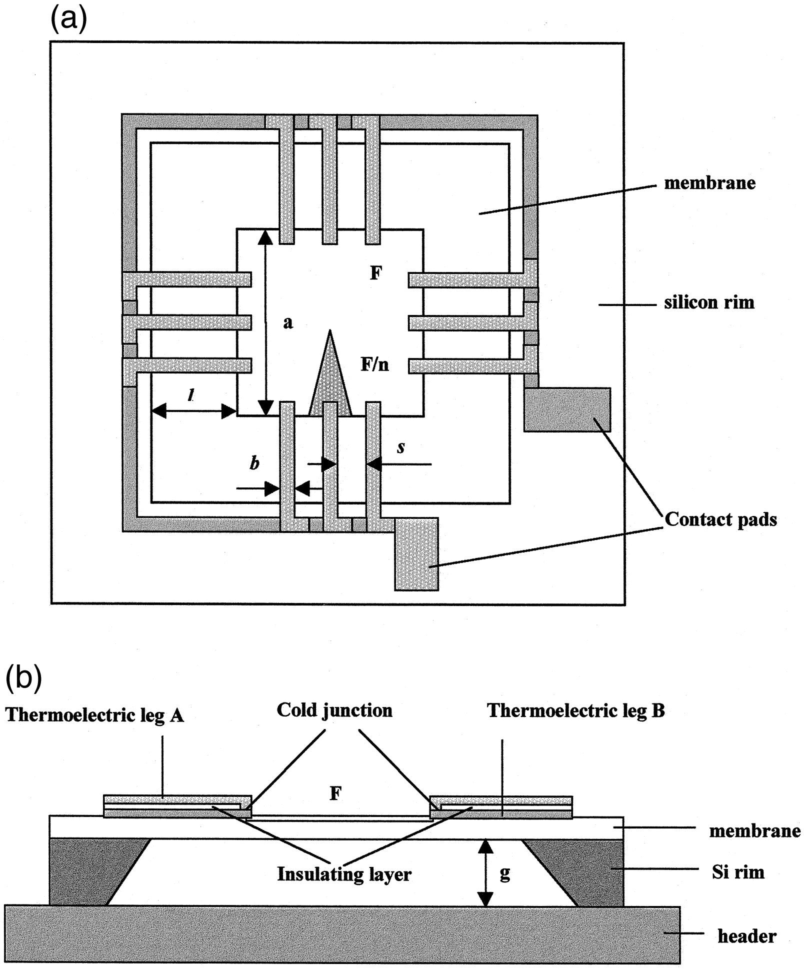

Fig. 1. Top view (1a) and cross-sectional view (1b) of a microelectromechanical thermoelectric cooler.

low thermal conductivity in order to achieve good thermal insulation of the cold junctions. The quadratic membrane results from the anisotropic etching of the silicon wafer. The bulk silicon rim acts as a heat sink. Heat is pumped laterally from the central region to the silicon substrate rim and then dissipated vertically through it to an external heat sink. The cooled area F is modelled as a quadratic area with the length a of the sides. Each thermocouple is a stack of two thermoelectric films (A and B, respectively) with an insulating layer between them (see Fig. 1b). The width of a thermocouple is b, its length (the distance between heat sink and cooled area F) is l and the spacing between thermocouples is s.

The modelling of the cooler can be carried out, in principle, by three-dimensional simulation tools. However, for the thin film device of Fig. 1, the analysis can be performed in terms of a one-dimensional model. Usually, the thickness of the thermoelectric films, of the membrane and the insulating film is in the order of 1 μm, whereas the thermocouple length is in the order of 1 mm. Therefore, temperature distributions in the thickness dimension can be ignored. Furthermore, because of the symmetric design of the cooler, only one separated thermocouple has to be analysed. Such a thermocouple represents a cantilever beam with a cooled area F/n at the tip of the beam. In such cantilever beams, the heat expansion can be described by only one coordinate.

Fig. 2 shows the cross-sectional view of the thermal model for such a single thin film thermocouple. We assume that the temperature T_c is uniform over the whole area F/n. This can be achieved by a metallization of F, which also reduces the absorption of thermal radiation and therefore minimizes the impact of heat from the ambient. Furthermore, heat is absorbed by the area F/n from the ambient due to conduction/convection of the surrounding gas. N represents an additional thermal load, for example by a microelectronic device which has to be cooled. The cold junction at the position $x=l$ generates the cooling power Q (Peltier ‘heat’), which is given by the Seebeck-coefficients of the legs (α_A and α_B, respectively), the current I and the temperature T_c

$$Q=(\alpha_A-\alpha_B)IT_c. \tag{1}$$

In the volume element dV of the cantilever beam heat is absorbed by radiation and convection from the ambient,

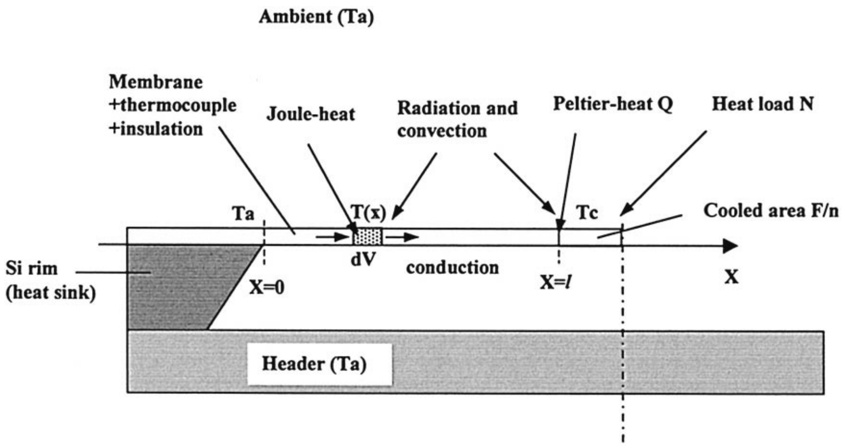

Fig. 2. Cross-sectional view of the thermal model.

Joule's heat is generated by the current I through the thermocouple and heat is conducted from the heat sink with ambient temperature T_a to the cold junction with temperature T_c. The heat balance equation for the volume element dV at position x with a temperature $T_c < T(x) < T_a$ is:

$$\lambda_t d_t b \frac{d^2(T(x) - T_a)}{dx^2} + \frac{I^2}{b}\left(\frac{\rho_A}{d_A} + \frac{\rho_B}{d_B}\right) - \left(8\varepsilon\sigma T_a^3 + 2\beta\right) b\left(T(x) - T_a\right) = 0. \quad (2)$$

Here, the first term describes the heat conduction through the cantilever beam, the second term is Joule's heat and the third term is the heat absorbed by radiation and convection with a heat transfer coefficient $\gamma = 8\varepsilon\sigma T_a^3 + 2\beta$. We assume that $(T(x) - T_a)/T_a \ll 1$ and we use the approximation $\varepsilon\sigma(T(x)^4 - T_a^4) \approx 4\varepsilon\sigma T_a^3(T(x) - T_a)$ for the radiation term. σ is the Stefan–Boltzmann constant, ε is the emissivity of the beam, β is the heat transfer coefficient for convection of the surrounding gas, ρ_A and ρ_B are the electrical resistivities, λ_A and λ_B are the thermal conductivities and d_A and d_B are the thicknesses of the thermoelectric legs. The term $\lambda_t d_t$ describes the total thermal conductance of the cantilever according to

$$\lambda_t d_t = \lambda_A d_A + \lambda_B d_B + \lambda_m d_m + \lambda_i d_i \quad (3)$$

where λ_m, d_m and λ_i, d_i denotes the thermal conductivity and thickness of the membrane and insulating film, respectively. The differential Eq. (2) can be solved by using the boundary conditions

$$(T(x) - T_a)|_{x=0} = 0 \quad (4)$$

$$\lambda_t d_t b \left.\frac{\mathrm{d}(T(x) - T_a)}{\mathrm{d}x}\right|_{x=l} = -(Q - N) - \gamma_F \frac{F}{n} \times (T(l) - T_a) \quad (5)$$

where $\gamma_F = 8\varepsilon_F \sigma T_a^3 + 2\beta$ denotes the heat transfer coefficient for radiation and convection and ε_F denotes the emissivity of the area F. The solution of Eq. (2) is

$$T(x) - T_a = \left(\frac{-(Q - N) - \gamma_F \frac{F}{n}(T_c - T_a)}{\lambda_t d_t b\sqrt{p}\cosh(l\sqrt{p})} - \frac{I^2 R \cdot \exp(-l\sqrt{p})}{lb\gamma\cosh(l\sqrt{p})}\right)\sinh(x\sqrt{p}) + \frac{I^2 R}{lb\gamma}\left(1 - \exp(-x\sqrt{p})\right) \quad (6)$$

where R denotes the resistance of the thermocouple and $p = \gamma/(\lambda_t d_t)$. Using Eq. (6) for the calculation of $T(x = l) - T_a = T_c - T_a$, we find

$$(T_c - T_a) = \left(\frac{\lambda_t d_t b\sqrt{p}}{\tanh(l\sqrt{p})} + \gamma_F \frac{F}{n}\right) = -(Q - N) + I^2 R \frac{\left(1 - \frac{1}{\cosh(l\sqrt{p})}\right)}{l\sqrt{p}\tanh(l\sqrt{p})}. \quad (7)$$

Here, the factor $G = \left(\frac{\lambda_t d_t b\sqrt{p}}{\tanh(l\sqrt{p})} + \gamma_F \frac{F}{n}\right)$ of $(T_c - T_a)$ represents the thermal conductance of the thin film device. The factor $C = \frac{\left(1 - \frac{1}{\cosh(l\sqrt{p})}\right)}{l\sqrt{p}\tanh(l\sqrt{p})}$ of Joule's heat represents the exchange of Joule's heat with the ambient and with the cold junction. With these designations, the heat balance equation

$$(T_c - T_a) \cdot G = -(Q - N) + I^2 R \cdot C = -(\alpha_A - \alpha_B) I T_c + N + I^2 R \cdot C \quad (8)$$

corresponds to the equation for a bulk thermoelectric cooler. However, for bulk coolers, the thermal conductance is given by $G=(\lambda_A l/W_A)+(\lambda_B l/W_B)$, where W_A and W_B are the cross-sections of the thermoelectric legs and $C=1/2$.

Using Eq. (8), we deduce the optimum current I_{opt}, which maximizes the temperature difference $T_c - T_a$ and the cooling power:

$$I_{opt} = \frac{(\alpha_A - \alpha_B) T_c}{2RC} \tag{9}$$

With I_{opt}, we calculate the maximum temperature difference

$$(T_c - T_a)_{max} \cdot G = -\frac{(\alpha_A - \alpha_B)^2 T_c^2}{4RC} + N. \tag{10}$$

Without any heat load N, the thin film device can achieve a maximum temperature difference

$$(T_c - T_a)_{max} = -\frac{(\alpha_A - \alpha_B)^2 T_c^2}{4RGC}. \tag{11}$$

The maximum heat load can be removed from the cooler for $(T_c - T_a)_{max} = 0$. Consequently, we deduce from Eq. (10):

$$N_{max} = \frac{(\alpha_A - \alpha_B)^2 T_a^2}{4RC}. \tag{12}$$

3. Results and discussion

We discuss the maximum temperature difference $(T_c - T_a)_{max}$ and the maximum heat load N_{max} for various operation conditions.

3.1. Minimum heat exchange by convection (operation in high vacuum)

For operation in high vacuum (pressure $< 10^{-3}$ mbar) the heat flux by convection can be neglected ($\beta = 0$). Then, we can find a practicable leg length l, for which the term $(l\sqrt{p}) \ll 1$. Since

$$l\sqrt{p} = l\sqrt{\frac{\gamma}{\lambda_t d_t}} = \sqrt{\frac{\gamma b l}{\lambda_t d_t b/l}} = \sqrt{\frac{8\varepsilon\sigma T_a^3 b l}{\lambda_t d_t b/l}}, \tag{13}$$

the condition $(l\sqrt{p}) \ll 1$ corresponds to a small thermal conductance by radiation in comparison with the thermal conductance by heat conduction. For $\varepsilon = 1$ (worst case!), $T_a = 293$ K, $d_A = d_B = 1$ μm, $d_S = 1$ μm and $\lambda_t d_t = \lambda_A d_A + \lambda_B d_B + \lambda_s d_s = 4.56 \times 10^{-6}$ W/K we calculate $(l\sqrt{p}) = l(1.58/\text{mm})$. Here, $\lambda_s d_s = \lambda_m d_m + \lambda_i d_i$ denotes the substrate's thermal conductivity and thickness, including the thermal conductivities and thicknesses of membrane and insulating film. Typical material properties, which we have used for calculations are represented in Table 1. For $l \leq 0.3$ mm and, consequently, $(l\sqrt{p}) \leq 0.5$ the approximations

$$\left(1 - \frac{1}{\cosh(l\sqrt{p})}\right) \approx \frac{(l\sqrt{p})^2}{2} \text{ and } \tanh(l\sqrt{p}) \approx (l\sqrt{p})$$

can be applied. With these approximations, the thermal conductance is

$$G = \frac{\lambda_t d_t b}{l} + \gamma_F \frac{F}{n} \tag{14}$$

the factor $C = 1/2$, and the maximum temperature difference can be expressed by

$$(T_c - T_a)_{max} = -\frac{(\alpha_A - \alpha_B)^2 T_c^2}{2R\left(\frac{\lambda_t d_t b}{l} + \gamma_F \frac{F}{n}\right)} = -\frac{(\alpha_A - \alpha_B)^2 T_c^2}{2\left(\frac{\rho_A}{d_A} + \frac{\rho_B}{d_B}\right)\left(\lambda_A d_A + \lambda_B d_B + \lambda_S d_S + \gamma_F \frac{Fl}{nb}\right)}. \tag{15}$$

In order to calculate the maximum temperature difference, we have to study the thermoelectric properties of thin

Table 1
Thermoelectric properties and film parameters used for calculations

Materials or geometrical parameters	at $T_c = 250$ K	at $T_a = 293$ K
Seebeck-coefficient $\alpha_A = -\alpha_B = \alpha$ (μV/K)	185	230
Electrical resistivity $\rho_A = \rho_B = \rho$ (10^{-5} Ω m)	1.33	1.70
Thermal conductivity $\lambda_A = \lambda_B = \lambda$ (W/m K)	1.28	1.08
Thermoelectric efficiency $z_A = z_B = z = \alpha^2/(\rho\lambda)$($10^{-3}$/K)	2.00	2.88
Emissivity ε, ε_F (worst case!)	1	1
Substrate's thermal conductivity λ_S (W/m K)	2.0	2.2
Length of the legs l (mm)	0.3	0.3
Lateral length of the cooled area a (mm)	1	1

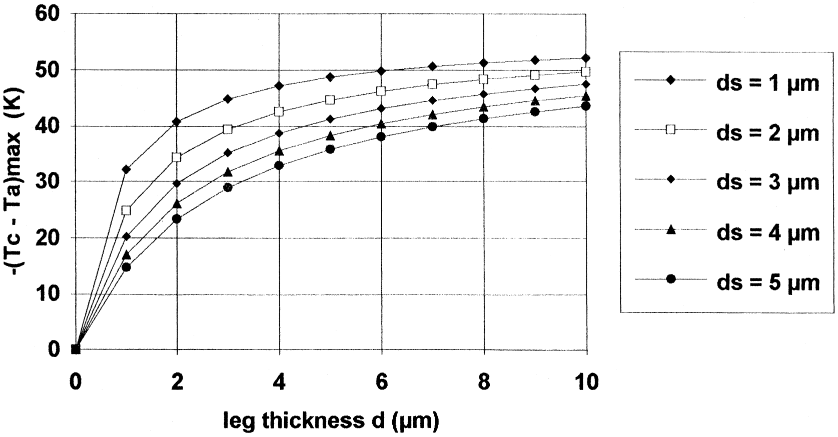

Fig. 3. Calculated maximum temperature difference as a function of leg thickness d and substrate thickness d_S.

film materials. p-type $(Bi_{0.5}Sb_{1.5})\ Te_3$-films show the best thermoelectric efficiency at room temperature. They have been prepared by flash evaporation [15] or MBE [16] and subsequent annealing. The properties of these optimized films are close to the bulk material and are represented in Table 1. The preparation of n-type films with a high figure of merit is much more complicated. Our modelling is based on the (somewhat optimistic) assumption of a high efficient n-type film with the same properties like the best p-type films. By further improvement of the preparation techniques, certainly it will be possible to realize such high efficient n-type films. Furthermore, the calculations are performed for identical leg thickness $d_A = d_B = d$. Then, the maximum temperature difference can be expressed as

$$(T_c - T_a)_{\max} = -\frac{zT_c^2}{2\left(1 + \dfrac{\lambda_S d_S}{2\lambda d} + \gamma_F \dfrac{Fl}{2nb\lambda d}\right)}. \qquad (16)$$

The leg width b is limited by the circumference $U = 4a$ of the cooled area. For a very small spacing $s \ll b$, the maximum leg width is given by $b_{\max} = U/n$. Using $b_{\max}$ and $F/U = a/4$, we learn that $(T_c - T_a)_{\max}$ is independent on b:

$$(T_c - T_a)_{\max} = -\frac{zT_c^2}{2\left(1 + \dfrac{\lambda_S d_S}{2\lambda d} + \gamma_F \dfrac{al}{8\lambda d}\right)}. \qquad (17)$$

Fig. 3 shows the calculated maximum temperature difference as a function of the leg thickness d and substrate thickness d_S, calculated according to Eq. (17) for $T_a = 293$ K with the film data at $T_c = 250$ K (temperature of the cold junction). It should be mentioned that in Eq. (17), the contact resistance of the thermocouples is neglected. Therefore, the temperature difference, which can be obtained in practice will be smaller than the calculated one. The curves of Fig. 3 represents the ultimate limits for thin film cooler with respect to the recent facilities of thermoelectric films. On the other hand, the contact resistance of such photolithographically patterned thin film devices is only a small part of the total resistance R. Therefore, the contact resistance will not drastically reduce the calculated curves.

Using Eq. (12) and the data of Table 1, we deduce the maximum heat load for a single thermocouple:

$$N_{\max} = \frac{4\alpha^2 T_a^2 bd}{2(\rho_A + \rho_B)l} = \frac{\alpha^2 T_a^2 bd}{\rho l} \qquad (18)$$

and the total heat load, removed by n thermocouples.

$$N = n \cdot N_{\max} = \frac{4\alpha^2 T_a^2 da}{\rho l}. \qquad (19)$$

For given dimensions of the cooled area ($a = 1$ mm) and of the leg length ($l = 0.3$ mm), N can be increased by increasing leg thickness d. This is due to an increase of the optimum current I_{opt} with increasing leg thickness. The optimum current and optimum current density, respectively, are given by

$$j_{opt} = \frac{I_{opt}}{bd} = \frac{(\alpha_A - \alpha_B)T}{2RCbd} = \frac{\alpha T}{\rho l} \qquad (20)$$

where we apply the temperature $T = T_c$ for the case of maximum temperature difference and $T = T_a$ for the case of maximum heat load. Using the data of Table 1 at $T_a = 293$ K, the maximum heat load and the corresponding current density of the thin film cooler are calculated and represented in Table 2.

Table 2
Maximum heat load N and optimum current density j_{opt} of the thin film cooler as a function of leg thickness d

Leg thickness d (μm)	Heat load N (mW)	j_{opt} (10^3 A/cm^2)
1	3.56	1.32
5	17.8	1.32
10	35.6	1.32

Table 3
$(T_c - T_a)_{max}$ and maximum heat load N as a function of leg thickness d for a leg length $l = 1$ mm, substrate thickness $d_S = 1$ μm and with $\gamma = \gamma_F = 100$ W/m^2 K

d (μm)	$(l\sqrt{p})$	$\tanh(l\sqrt{p})$	$(1 - \frac{1}{\cosh(l\sqrt{p})})$	$(T_c - T_a)_{max}$ (K)	j_{opt} (10^2 A/cm^2)	N (mW)	j_{opt} (10^2 A/cm^2)
1	4.68	1.000	0.981	−10.3	9.20	2.50	9.28
2	3.75	0.999	0.953	−14.4	7.27	4.01	7.43
3	3.21	0.997	0.919	−16.8	6.15	5.15	6.36
4	2.86	0.994	0.886	−18.4	5.46	6.11	5.67
5	2.60	0.989	0.852	−19.6	4.94	6.95	5.15

3.2. Maximum heat flux by convection (operation at normal pressure of the surrounding gas)

By using the microcooler in a normal atmosphere, heat flux by convection has to be involved. Usually a microcooler chip is attached on a header (see Fig. 1). Applying 4-in. silicon wafers, the distance g between membrane and header is about 500 μm. Then, the heat transfer coefficient β for convective heat flux between membrane and header can be expressed by $\beta = \lambda_{gas}/g$, where λ_{gas} denotes the thermal conductivity of the surrounding gas ($\beta = 52$ W/m^2 K for air). Furthermore, free convection on the other side of the cantilever beam and thermal radiation has to be involved. Therefore, $\gamma = \gamma_F \approx 100$ W/m^2 K is a reasonable value for operation at normal atmosphere. Using this value, we calculate the terms $(l\sqrt{p})$, $\tanh(l\sqrt{p})$ and $(1 - \frac{1}{\cosh(l\sqrt{p})})$ for a leg length $l = 1$ mm (Table 3).

We learn from Table 3 that below a leg thickness of 4 μm the term $(l\sqrt{p}) \geq 3$ and the terms $\tanh(l\sqrt{p})$ and $(1 - \frac{1}{\cosh(l\sqrt{p})})$ can be approximated by unity. Therefore, we deduce from Eq. (7) with the designations of Section 3.1

$$(T_c - T_a)\left(\lambda_t d_t b\sqrt{p} + \gamma_F \frac{F}{n}\right) = -(Q - N) + I^2 R \frac{I}{(l\sqrt{p})} \quad (21)$$

and with $\gamma = \gamma_F$ for the maximum temperature difference

$$(T_c - T_a)_{max} = -\frac{zT_c^2}{4\left(1 + \frac{\lambda_S d_S}{2\lambda d}\right)\left(1 + \frac{a\sqrt{p}}{4}\right)}. \quad (22)$$

Table 3 shows also the maximum temperature difference (for $d_S = 1$ μm) and the corresponding optimum current density

$$j_{opt} = \frac{I_{opt}}{bd} = \frac{(\alpha_A - \alpha_B)T}{2RCbd} = \frac{\alpha T\sqrt{p}}{2\rho} \quad (23)$$

calculated with the parameters of Table 1 at $T = T_c$. Furthermore, the maximum heat load (for $T_c - T_a = 0$)

$$N = n \cdot N_{max} = \frac{2\alpha^2 T_a^2 ad\sqrt{p}}{\rho} \quad (24)$$

and the corresponding optimum current density, calculated with the parameters of Table 1 at $T = T_a$, are shown in Table 3. The results demonstrate that a microcooler using thermoelectric films with $z = 2.00 \times 10^{-3}$/K can perform a maximum temperature difference of about 20 K at normal atmosphere. Therefore, e.g., dew-point sensors based on such microelectromechanical coolers can be realized by batch-process fabrication.

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Friedemann Völklein received both his BS and DS degrees in physics from the University of Jena (Germany). In 1974, he became a scientific coworker of the Physical–Technical Institute Jena. He specializes in solid-state physics of thin films and their applications in thermoelectric microsensors. In 1990, he became head of the sensor department of the Physical–Technical Institute Jena and taught solid-state physics at the University of Karlsruhe. Since 1991, he has been senior scientist of ETH's Physical Electronics Laboratory (Zürich), where he concentrates on research and development of CMOS-compatible microsensors, using the facilities of ABB Corporate Research microlaboratory. Since 1992, he has been professor of Physical Technologies of FH Wiesbaden, University of Applied Sciences. He is author or co-author of over 60 publications in scientific or technical journals and 13 patents.

Michael Rowe holds University of Wales BS degrees in both Pure Mathematics (1964) and Physics (1965) and a PhD (1968). In 1988, he was awarded a Doctor of Science for his contributions to the development of improved thermoelectric materials. He has held successive positions of United Kingdom Atomic Energy Research Fellow, Lecturer and Reader at the School of Engineering University of Cardiff, Wales and in 1994 was awarded a Personal chair in Electronic Engineering. Currently, Professor Rowe is Director of the NEDO Laboratory for Thermoelectric Engineering in the School of Engineering, Cardiff University, and Deputy Head of the Electronics Division. He was a recipient of a British Gas Research Fellowship on two occasions (1977) and (1988)—the only UK researcher to do so. In 1989, he received the outstanding technical paper award with Professor D.V. Morgan and Dr. J. Keily at the Eighth International Conference on Thermoelectric Energy Conversion, Nancy, France and in 1990 was runner-up for the British Electronics Week research activity of the year award. Professor Rowe has published more than 200 research papers and authored or co-authored three books on thermoelectrics and compiled and edited the CRC Handbook of thermoelectricc—the fist definitive text on this subject. In 1993, he was a European–Japanese visiting professor to the EEC laboratory Tsukuba and in 1994, a visiting professor to Centro Tecnico Aerorpacial, Brazil. Professor Rowe is a Fellow of the Institute of Physics—and off the Institution of Electrical Engineers. He is President of the International Thermoelectric Society and Deputy President of the European Thermoelectric Society.

Gao Min received his BS from Xidan University, Xian, China in 1982 and PhD from Cardiff University, Cardiff, UK in 1996. His research interests include thermoelectric materials, devices and applications, transport properties of semiconductor materials, semiconductor surface analysis. He is author or co-author of over 50 publications and one book.